Alizarin

72-48-0 | DTXSID5045960

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 1350 L/kg

Global applicability domain: Inside

Local applicability domain index: 4.25e-01

Confidence level: 6.47e-01

Nearest Neighbors from the Training Set

Image not found
1-Amino-2-methylanthraquinone
Measured: 7940
Predicted: 4960

Image not found
Flutriafol
Measured: 75.9
Predicted: 510

Image not found
Anthraquinone
Measured: 3720
Predicted: 2300

Image not found
2-Acetylaminofluorene
Measured: 1380
Predicted: 1860

Image not found
9-Anthracenecarboxylic acid
Measured: 550
Predicted: 1400